

603135

Transport in Carbon Nanotubes

S. DATTA and YONGQIANG XUE

Purdue University
West Lafayette, IN

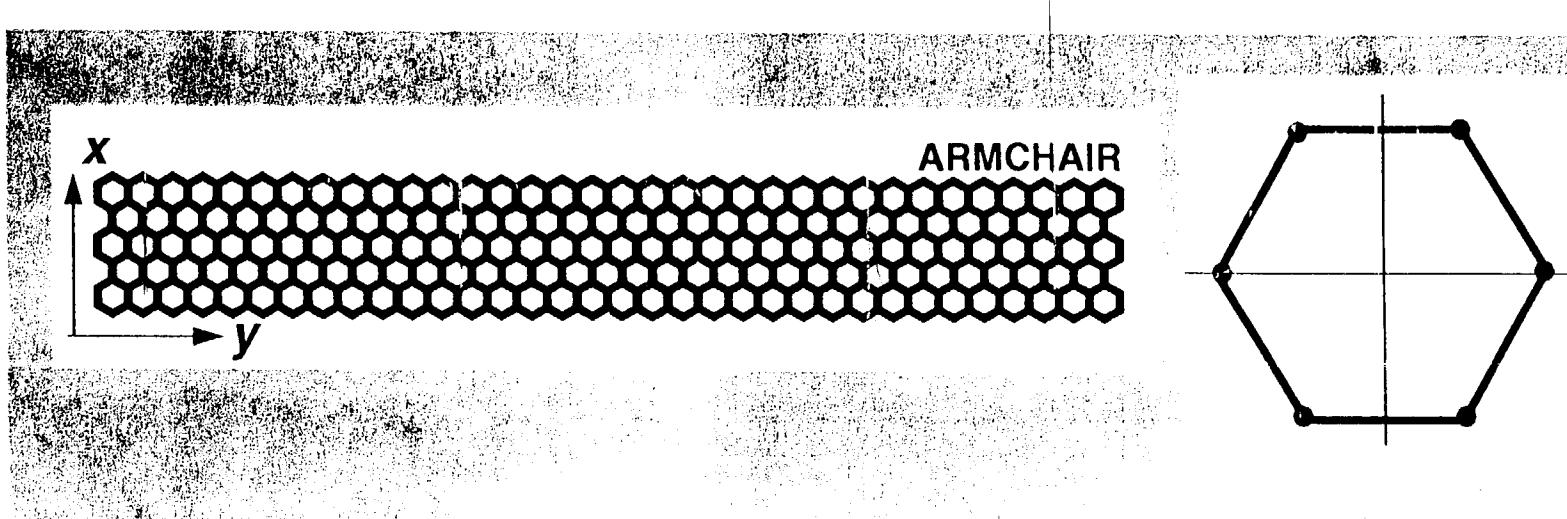
M. P. ANANTRAM

NASA Ames Research Center
Moffett Field, CA

MOTIVATION & OUTLINE

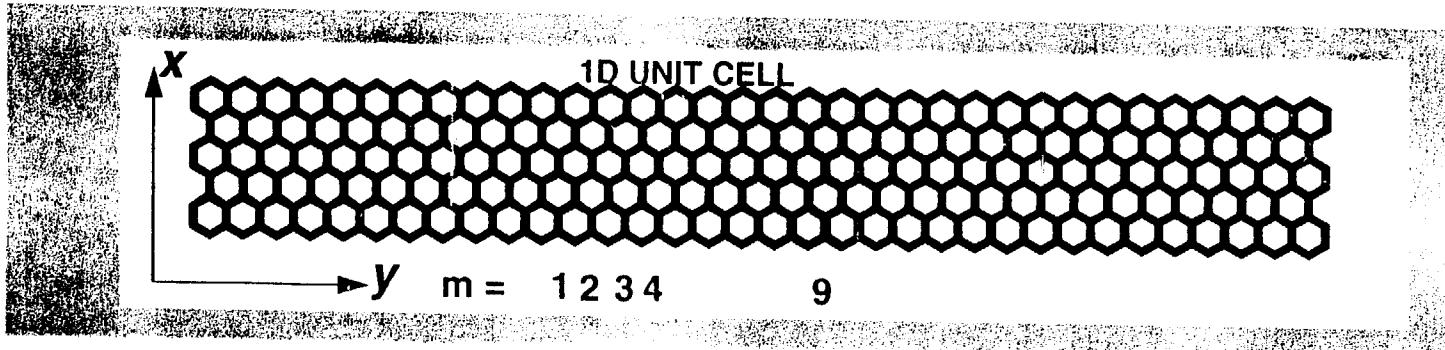
- Coupling between CNT and simple metals (FEG)
- Coupling between a graphene sheet and FEG
- What happens when the sheet----->strip (CNT)
- Dependence of coupling on width of strip and disorder

GRAPHENE STRIP IN UNIFORM CONTACT WITH METAL



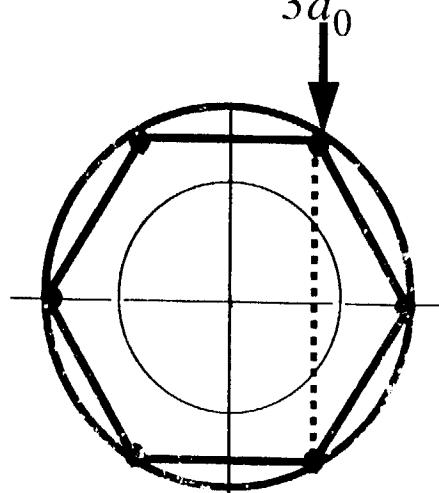
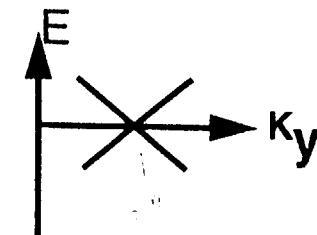
- K_y is conserved
- K_x conservation is relaxed due to finite *width* of *contact area*
- FEG couples better to CNT than to graphene
- Cut-off K_{Fermi} of metal is smaller than $\frac{4\pi}{3a_0} = 1.7 \text{ \AA}^{-1}$

COUPLING TO ARMCHAIR TUBES

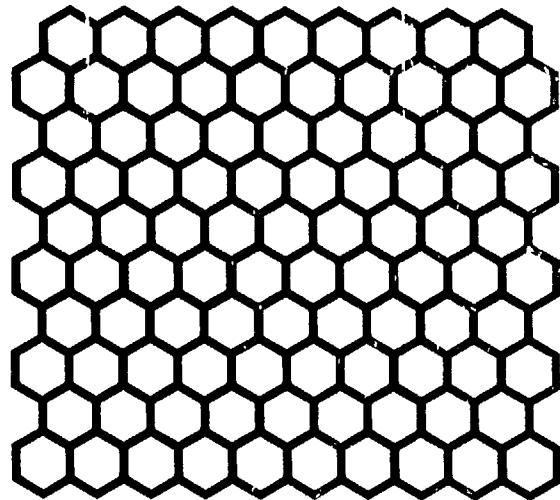


$$\Psi = e^{imk_y a_0} \phi \quad m = \text{integer and } \phi \text{ is wave func. of atoms in 1D unit cell}$$

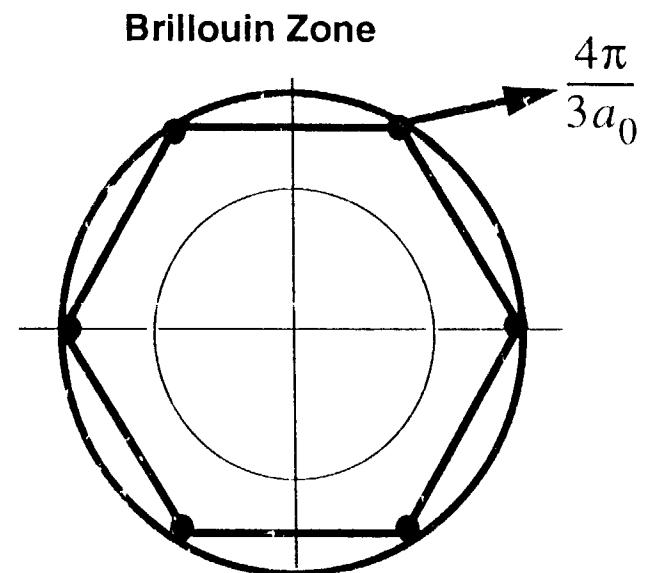
- $E=0$ at $K_y = \frac{2\pi}{3a_0} = 0.85 \text{ \AA}^{-1}$
- Metal with $K_{\text{Fermi}} < \frac{2\pi}{3a_0}$ couples weakly



GRAPHENE SHEET IN UNIFORM CONTACT WITH METAL



FEG
(Free Electron Gas)



For good coupling: Metal $K_{\text{Fermi}} > \frac{4\pi}{3a_0}$

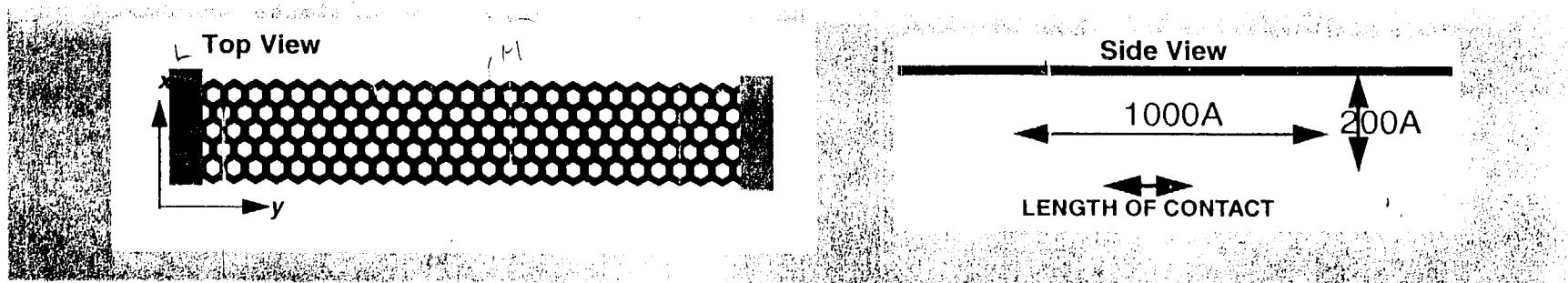
K-vector along plane is not conserved for most metals
Poor coupling.

	$K_{\text{Fermi}} \text{ \AA}^{-1}$
Cs	0.65
Ag	1.20
Au	1.21
Hg	1.37
Al	1.75
Graphene	1.7

* Ashcroft & Mermin, Solid State Physics

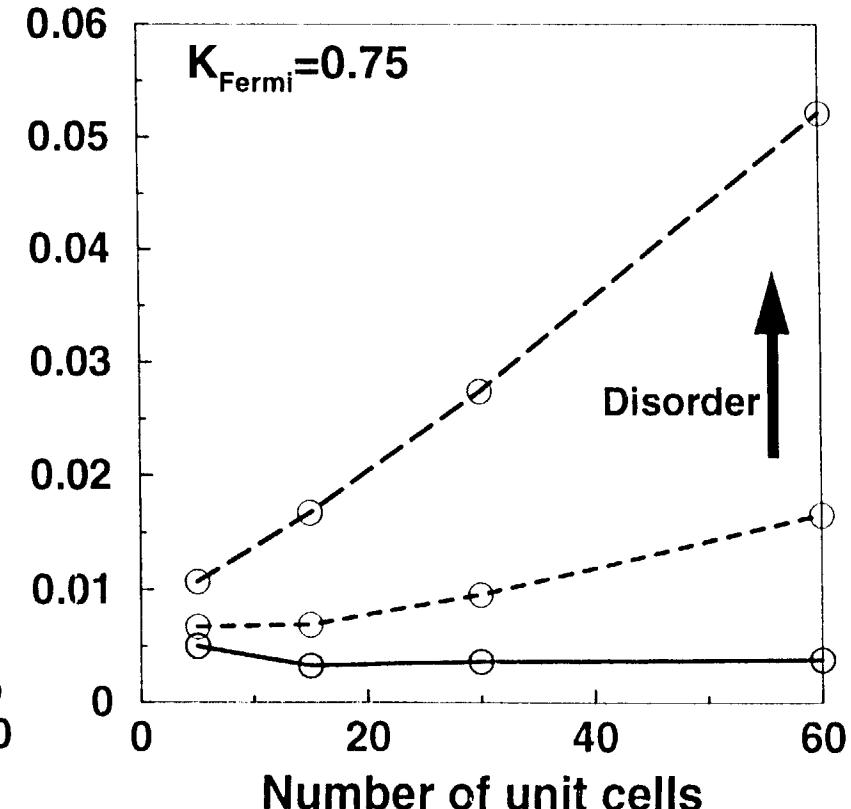
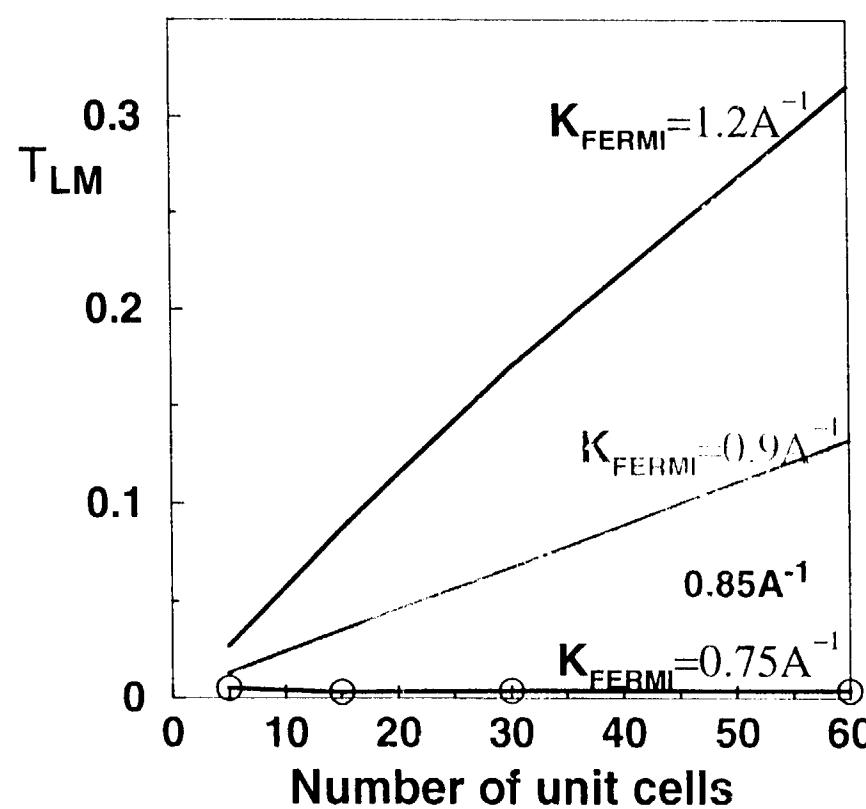
EFFECT OF HIGHER SUBBANDS ON dI/dV VERSUS V

- **S. Frank, P. Poncharal, Z. L. Wang & W. A. de Heer, Science, v.280 (1998)]**

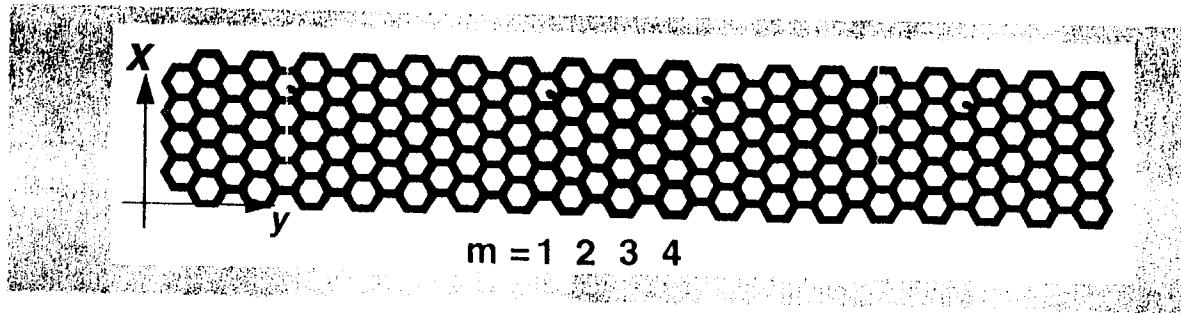


- Anantram & Govindan, Transport through carbon nanotubes with defects, Phys. Rev. B v.58 (1998);
- Compute self energy due to: (i) metal & (ii) semi-infinite CNT leads

~~$$T_{LM} = \text{Tr} [E_M G_d^r \Gamma_L G_d^a]$$~~

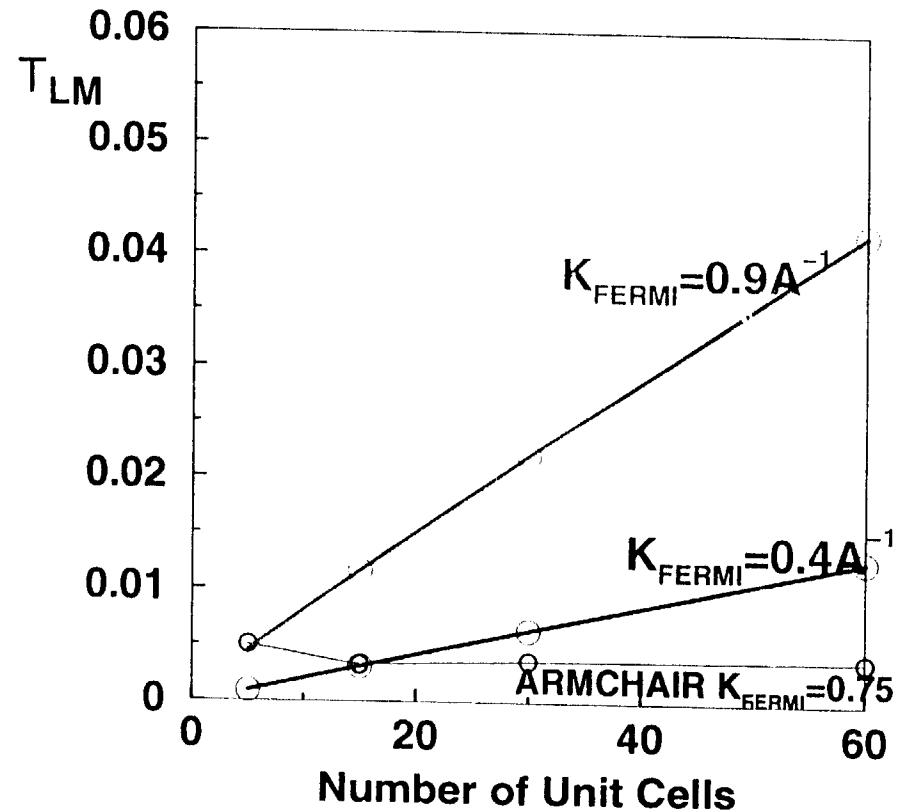
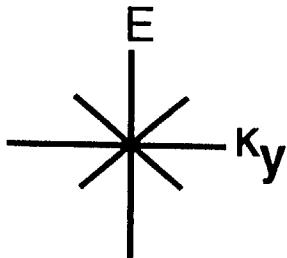


COUPLING TO ZIGZAG TUBES

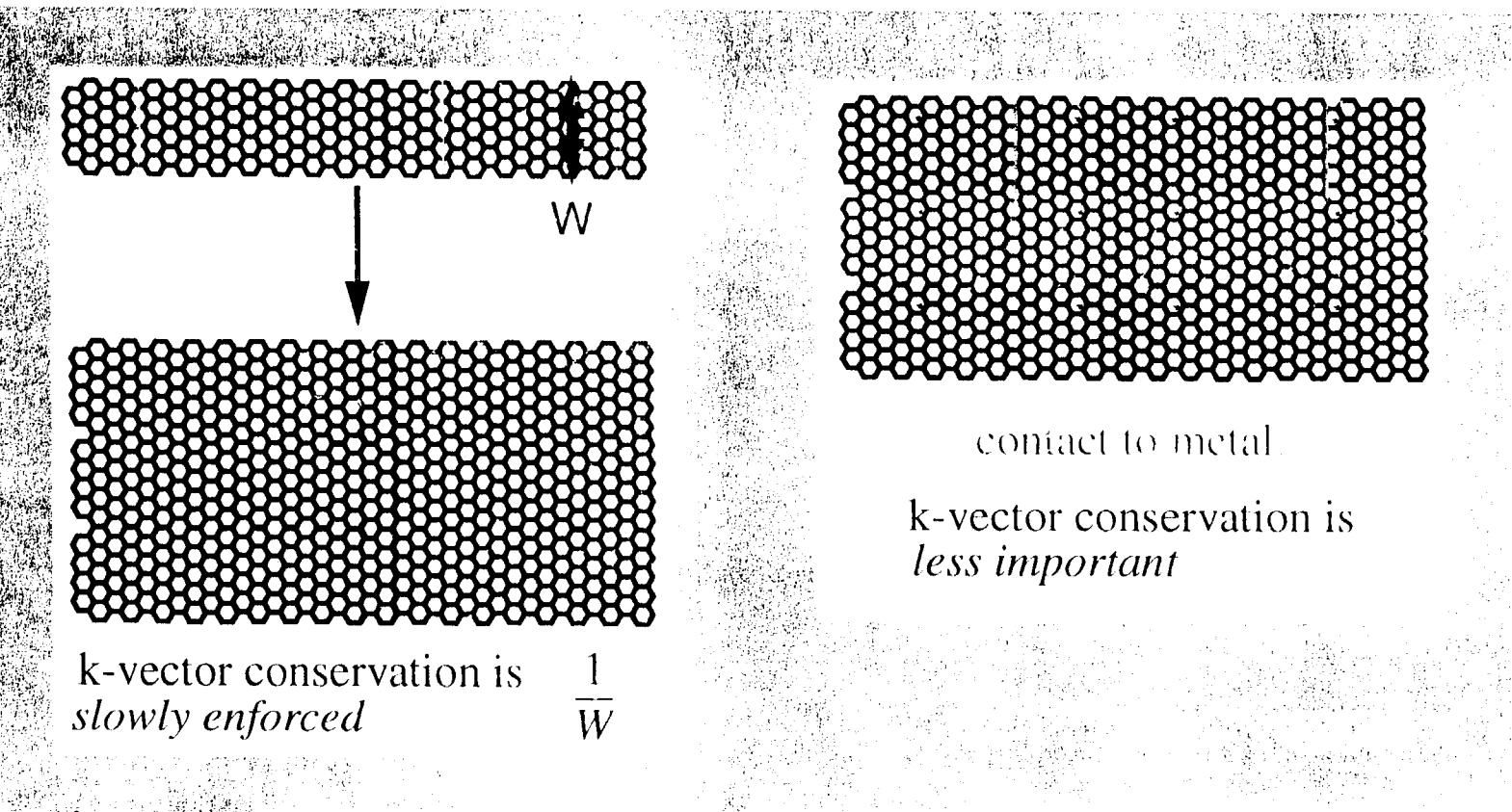


$$\Psi = e^{imK_y \sqrt{3}a_0} \phi$$

- $E=0$ at $K_y=0$.
- No cut-off value of metal K_{Fermi}



LARGE DIAMETER TUBES



- *Increase Transmission:* Small phase coherence length in metal / disorder in metal-CNT coupling [Frank et.al, Science, v.280 (1998)]

CONCLUSIONS

- Graphene sheet; does not couple well to most simple metals (K-vector conservation; $4\pi/3a_0$)
- CNT / graphene strip: couples much better to simple metals (need for k-vector conservation along width is relaxed)
- Axial k-vector conservation is still required. Causes non trivial difference in coupling of zigzag and armchair tubes to a FEG.

ARMCHAIR

$$\text{cut-off } K_{\text{Fermi}} = 2\pi/3a_0 = 0.85 \text{\AA}^{-1}$$

ZIGZAG

$$\text{cut-off } K_{\text{Fermi}} = 0$$

- Transmission increases with length of contact
- Disorder / small phase coherence length will increase transmission